Optimization, Linear Algebra, and a Little Bit of HOPE

LTE Review (September 2005 – January 2006)

January 17, 2006

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Optimization and Uncertainty Estimation (1411)

(8962 intern in 2001)

SAND2006-0759P

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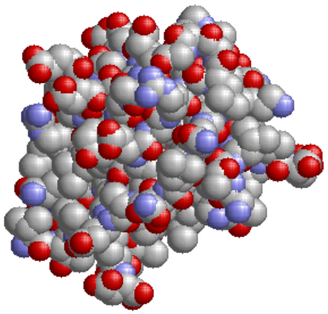
Outline

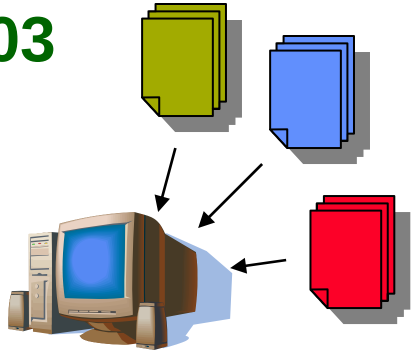
- **Biography**
- **DAKOTA (Optimization)**
  - Research and Product Impact
  - Collaborators: Mike Eldred, Bill Hart
- **Space-Time Preconditioners (Linear Algebra)**
  - Research
  - Collaborator: Andy Salinger
- **HOPE**
  - Future Impact
- **Other Contributions**

Biography

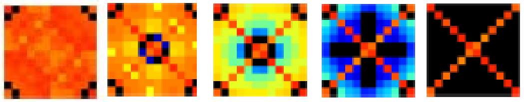
- **Ph.D., University of Maryland, August 2005**
  - *Advisor:* Dianne O’Leary
  - Homotopy Optimization Methods and Protein Structure Prediction



- **M.S., University of Maryland, December 2003**
  - *Advisor:* Dianne O’Leary
  - QCS: An Information Retrieval System for Improving Efficiency in Scientific Literature Searches



- **M.S., Western Michigan University, April 2001**
  - *Advisor:* Niloufer Mackey
  - Structure Preserving Algorithms for Perplectic Eigenproblems



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DAKOTA

- **Research Contributions**
  - Constraint relaxation for surrogate-based optimization (SBO) [M. Eldred]
  - **Goal:** Balance feasibility and optimality satisfaction within infeasible regions
  - **Contributions:**
    - Prototyped algorithm → production code
    - Identification of algorithmic enhancements
  - **Target:** Simulation-based optimization
  - **Impact:** *External customers*, design optimization, MEMS

- **Product Contributions**
  - Testing, documentation, COLINY [B. Hart]

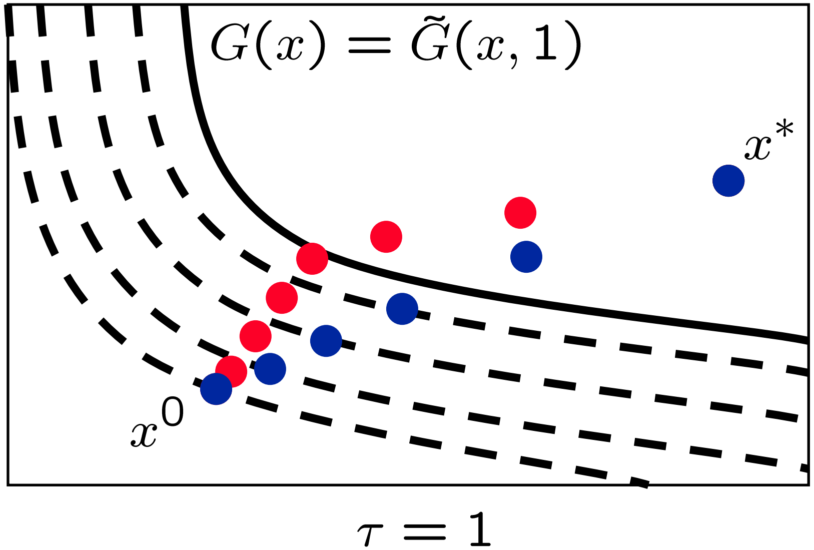
DAKOTA – Constraint Relaxation

Original	● Surrogate	● Relaxed
min $f(x)$	min $F(x)$	min $F(x)$
s.t. $g_l \le g(x) \le g_u$	s.t. $g_l \le G(x) \le g_u$	s.t. $g_l \le \tilde{G}(x) \le g_u$
$h(x) = 0$	$H(x) = 0$	$\tilde{H}(x) = 0$
$x_l \le x \le x_u$	$x_l \le x \le x_u$	$x_l \le x \le x_u$

$$\tilde{G}(x,\tau) = G(x) + (1-\tau)b_G$$
$$\tilde{H}(x,\tau) = H(x) + (1-\tau)b_H$$

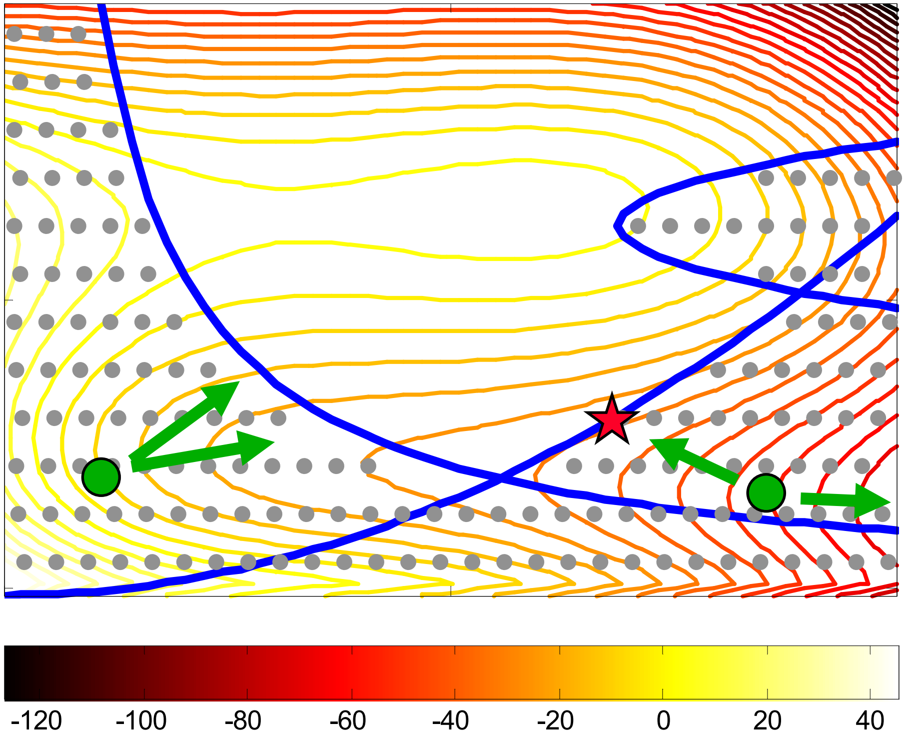
b_G, b_H chosen s.t.

$$g_l \le \tilde{G}(x^0, 0) \le g_u$$
$$\tilde{H}(x^0, 0) = 0$$

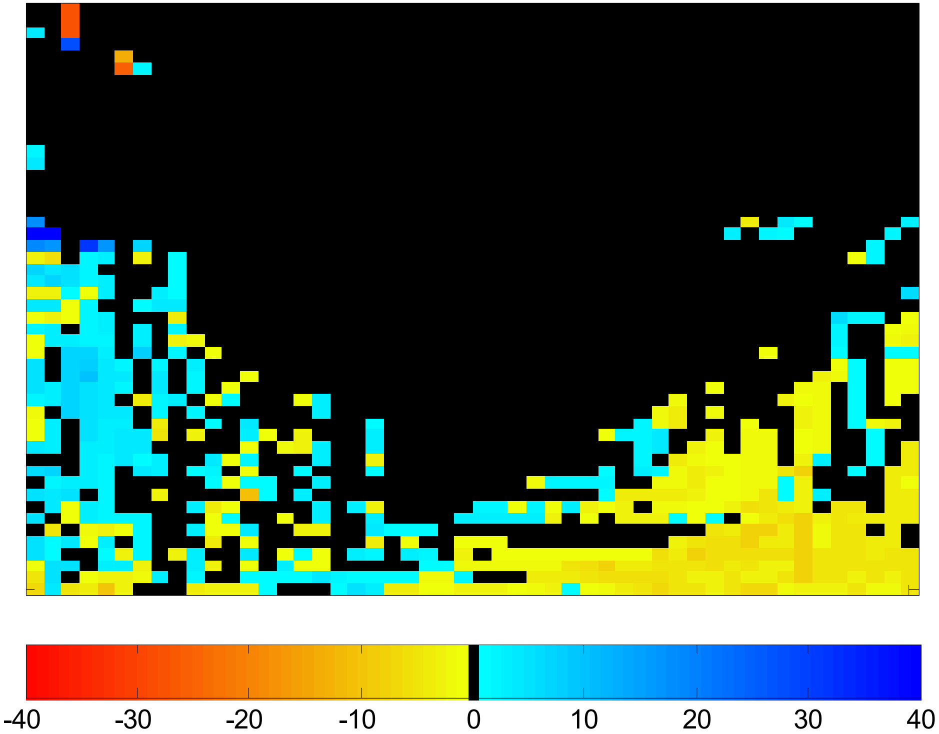


DAKOTA – Constraint Relaxation

Barnes Function



SBO Iteration Differences (True-Relaxed)

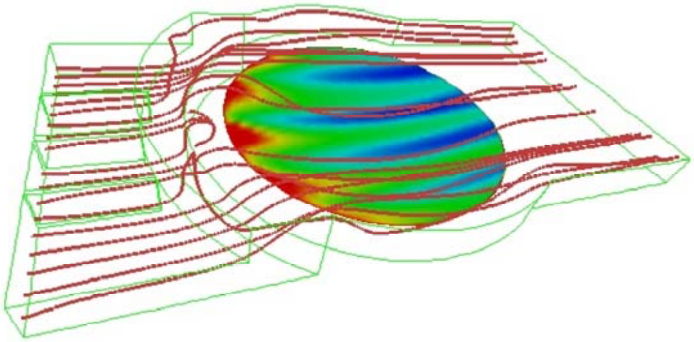


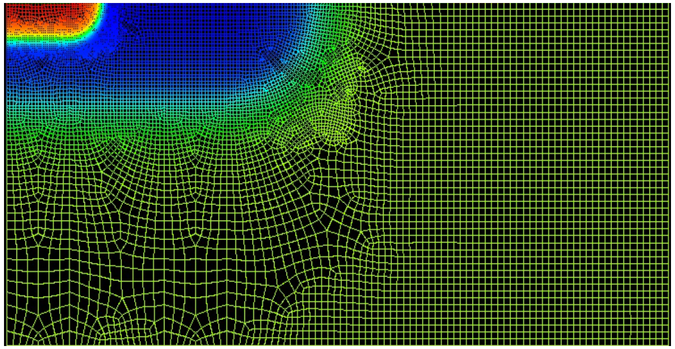
Using true constraints is better

Using relaxed constraints is better

Space-Time Preconditioners

- **Research Contributions**
  - Preconditioners for space-time formulations of transient problems [A. Salinger]
  - **Goal:** Efficiently solve (large) space-time problems
  - **Benefits:**
    - Achieve parallelism in time (and space)
    - Find initial values for particular solutions
    - More computation for parameter continuation
  - **Contributions:**
    - Implementation of preconditioner framework
    - Development of 4 preconditioners
    - Tutorial example
  - **Target:** Reacting fluid flows
  - **Impact:** MPSalsa, QASPR (Charon), Aria





Space-Time Preconditioners

Transient Simulation of: $\mathbf{B}\dot{\mathbf{x}} = \mathbf{f}(\mathbf{x}, \lambda)$

First solve: $\mathbf{B}\frac{\mathbf{x}_1 - \mathbf{x}_0}{\Delta t} - \mathbf{f}(\mathbf{x}_1, \lambda) = 0$

Then solve: $\mathbf{B}\frac{\mathbf{x}_2 - \mathbf{x}_1}{\Delta t} - \mathbf{f}(\mathbf{x}_2, \lambda) = 0$

Then solve: $\mathbf{B}\frac{\mathbf{x}_3 - \mathbf{x}_2}{\Delta t} - \mathbf{f}(\mathbf{x}_3, \lambda) = 0$

Instead, solve for all solutions at once: $\mathbf{g}(\mathbf{y}, \lambda) = 0$

where

$$\mathbf{y} = [\mathbf{x}_1 \ \mathbf{x}_2 \ \cdots \ \mathbf{x}_n]^T$$

$$\mathbf{g}_i = \mathbf{B}\mathbf{x}_i - \mathbf{B}\mathbf{x}_{i-1} - \Delta t \mathbf{f}(\mathbf{x}_i, \lambda)$$

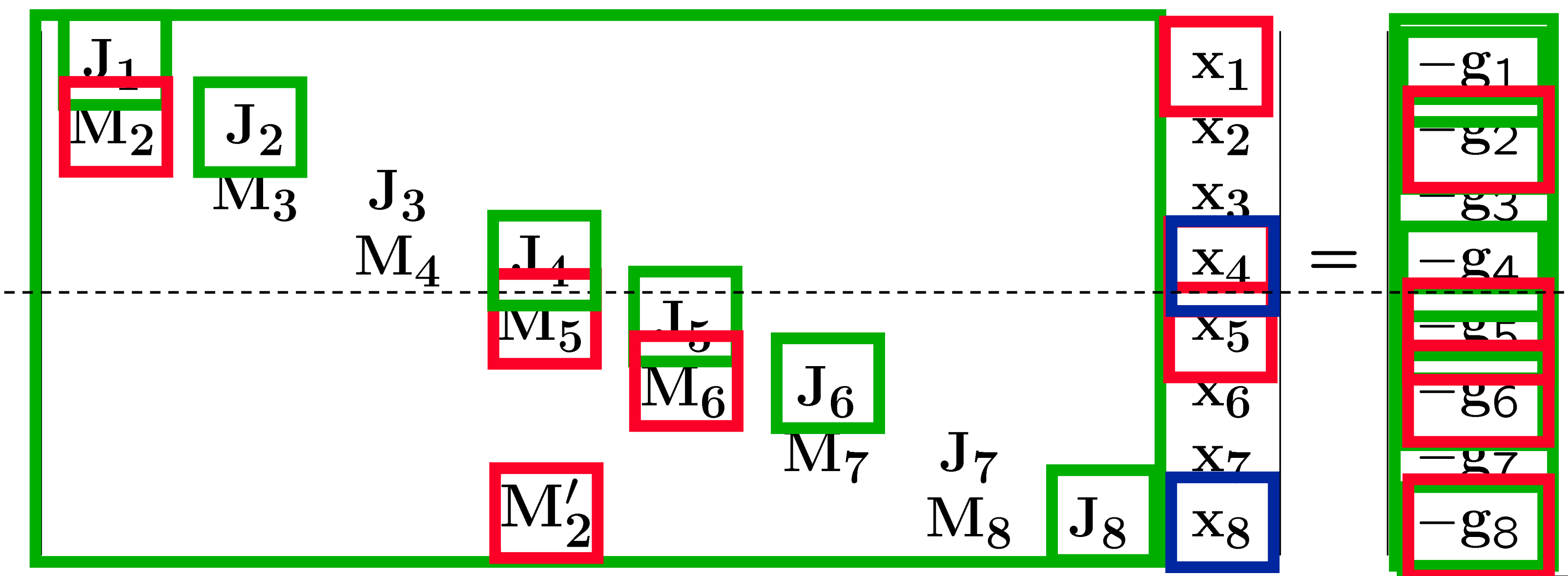
… and with Newton solve:

$$\begin{vmatrix} (\mathbf{B} - \Delta t \mathbf{J}) & 0 & 0 & 0 & 0 \\ -\mathbf{B} & (\mathbf{B} - \Delta t \mathbf{J}) & 0 & 0 & 0 \\ 0 & -\mathbf{B} & (\mathbf{B} - \Delta t \mathbf{J}) & 0 & 0 \\ 0 & 0 & -\mathbf{B} & (\mathbf{B} - \Delta t \mathbf{J}) & 0 \\ 0 & 0 & 0 & -\mathbf{B} & (\mathbf{B} - \Delta t \mathbf{J}) \end{vmatrix} \begin{vmatrix} \Delta \mathbf{x}_1 \\ \Delta \mathbf{x}_2 \\ \Delta \mathbf{x}_3 \\ \Delta \mathbf{x}_4 \\ \Delta \mathbf{x}_5 \end{vmatrix} = \begin{vmatrix} -\mathbf{g}_1 \\ -\mathbf{g}_2 \\ -\mathbf{g}_3 \\ -\mathbf{g}_4 \\ -\mathbf{g}_5 \end{vmatrix}$$

Space-Time Preconditioners

= Solve
$(J_i^{-1} g_i)$

= Mult, Add
$(-g_i - M_i x_{i-1})$



HOPE for Global Optimization

Original

$$\min_{x \in \mathbb{R}^n} \quad f(x)$$

Homotopy Optmization

$$\min_{x \in \mathbb{R}^n, \lambda \in \mathbb{R}} \quad F(x, \lambda), \qquad F(x, \lambda) = \begin{cases} e(x), & \lambda = 0 \\ f(x), & \lambda = 1 \end{cases}$$

- $F(x, \lambda)$ is a continuous deformation of $e(x)$ into $f(x)$
- Leverage known information about $e(x)$ (e.g., global minimizer)

- **Applications**
  - Successfully finds minimizers of several protein energy models
  - Standard global optimization test problems
- **Future Directions**
  - Constrained problems (function homotopy + constraint relaxation)
  - Homotopies on models
  - Sandia applications (param. estimation, multiscale, multiphysics)

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Other Contributions

• Funding

1) Co-PI (T. Kolda, B. Hart), "Derivative-Free Methods for Local and Global Optimization," *3-year MICS Proposal*, Dec. 2005.
2) Co-PI (T. Bauer), "Extending Retrieval and Analysis Capabilities in STANLEY using Multilinear Algebra Tools," *in preparation.*

• Publications

1) HOPE: A Homotopy Optimization Method for Protein Structure Prediction (D. O'Leary, D. Klimov, D. Thirumalai), *J. Comput. Biol.*, 12(10):1275-1288. Dec. 2005.
2) Homotopy Optimization Methods for Global Optimization (D. O'Leary), SAND2005-7495. Dec. 2005.
3) Formulations for Surrogate-Based Optimization with Data Fit, Multifidelity, and Reduced-Order Models (M. Eldred) , *in preparation*.
4) QCS: A Tool for Querying, Clustering and Summarizing Documents (D. O'Leary, J. Conroy), *in preparation*.
5) Global Optimization of a Simplified Protein Energy Model, *in preparation*.

• Presentations

1) Homotopy Optimization Methods, *Copper Mountain Conference on Iterative Methods*, Apr. 2006.
2) Preconditioners for Space-Time Systems, *SIAM Conference on Parallel Processing*, Feb. 2006.

• Service

- Grader, *Go Figure!* [C. Phillips]
- Journal Referee, *SIAM Review (1)*

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Thank You

Questions?